CHEM 2P20 SciFinder-n Exercise

The objective of this exercise is to gain experience exploring the chemical literature; register and use Brock's SciFinder-n database; learn how to create citations using ACS Style; explore chemical naming, structure drawing, reaction and database searching strategies; and, be better informed of Brock University chemists' research interests, productivity and expertise.

Go to the Brock Library Chemistry Research Guide to identify most-often used open and proprietary books/ebooks, web resources and scholarly databases. https://researchguides.library.brocku.ca/CHEM

Go to the SciFinder-n database link under the Chemistry Research Guide articles tab or the Brock Library list of databases and click on "register" for an account. This requires you to move through the Brock proxy server and create a unique SciFinder-n username and password. This registration is time limited so follow up with email authentication asap. This account is yours and is different from your Brock proxy username/password. Once you have an account for SciFinder-n remember to use your Brock proxy username/password and then your unique SciFinder-n username/password to access this database. This SciFinder-n access is yours as long as you are a member of the Brock University community.

Go to the Chemistry Department web site to review faculty and their research group's publications and activities. https://brocku.ca/mathematics-science/chemistry/directory/

Select **one** of the following Brock Department of Chemistry faculty member that specializes in organic chemistry from the following names: **Dudding, Duncan, Metallinos, Atkinson, Yan, or Zelisko**. Scan these faculty research groups' web site, list of publications, profile, review their interests, and do a bit of browsing before selecting your faculty member for this assignment.

Complete these ten questions using this form to get you thinking about scholarly research, chemistry and adding value to your learning.

I have chosen Dr. Pilkington for this example, answers in red.

Add your name and student number: _____

1. Name the researcher to be used for this exercise writing out variations in the spelling of their first/last name and/or initials that are often used in publications (this is really important!).

   Pilkington, Melanie or Pilkington, M.

   Does this researcher have an ORCiD iD? https://orcid.org/

   Yes/no (If so please include the ORCiD URL and link, note whether it is open to the public as well)
   https://orcid.org/0000-0002-9274-8512

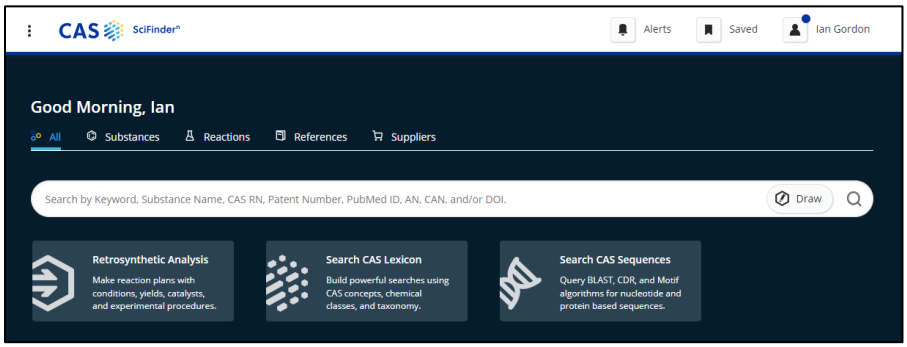
   Yes, open to the public.

   Have you registered/created a personal ORCiD ID? If yes, indicate below, if not, do it today, it is free and list below!
   https://orcid.org/0000-0003-1128-3301

2. Consult this faculty members research interests and publications to document keywords and phrases that best describe 1) chemistry subject areas / topics researched 2) substances/types/classes of chemical compounds investigated and 3) varying instrumentation, experimental equipment used as it relates to bio/synthetic/organic chemistry:

1. **Coordination Chemistry, Inorganic Chemistry, Organometallic Chemistry, Molecular Magnetism, Superconductivity**
2. **N-Heterocyclic compounds, Quinoline complexes, MOFs, SIMs, Thin films, Ligands, and TTF substituents**
3. **X-ray crystallography, X-ray diffraction, NMR, UV, EPR, and ESR spectroscopy**

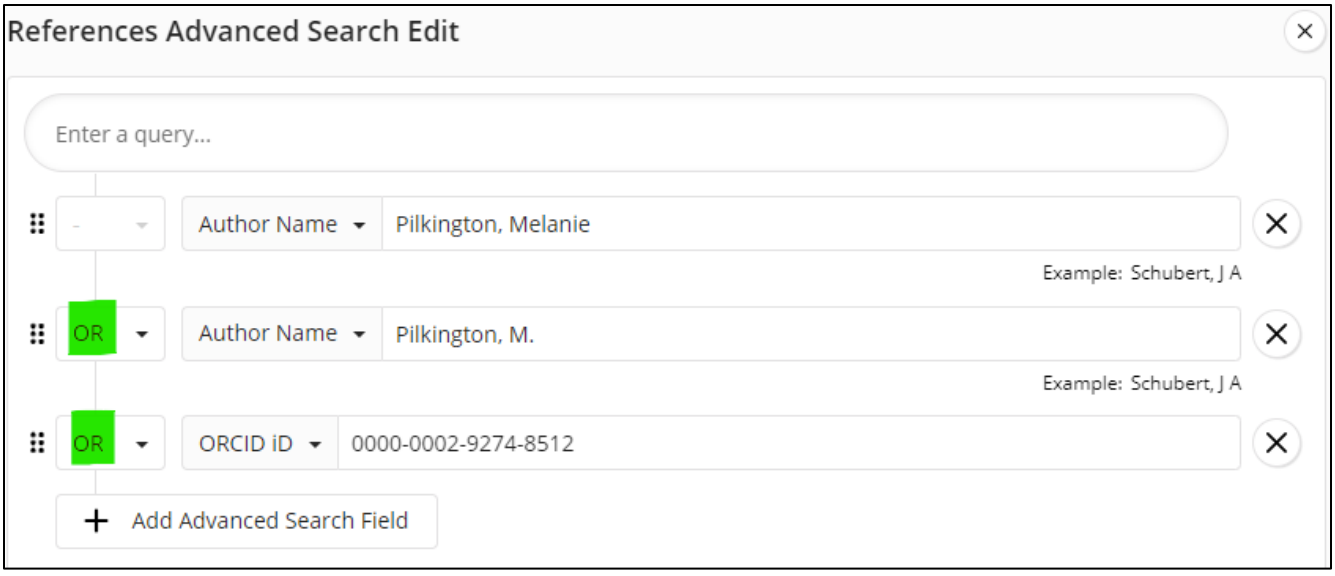
3. Follow instructions on the Brock *Library Chemistry Research Guide* under the "Articles" tab to register for a SciFinder-n account, confirm registration by e-mail authentication, and sign into the SciFinder-n database. Create a screen shot of your SciFinder-n account search engine page below that includes your personal name located on this databases entry point to confirm that you have an account: (Here is mine)



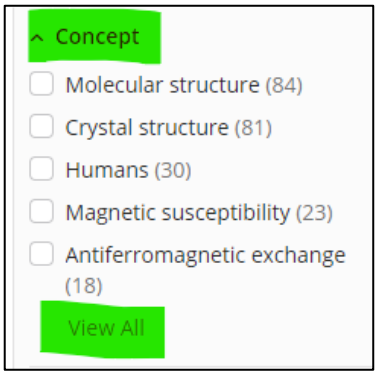
Check out the following SciFinder-n Training resources (you don't need to log in to view these).

4. Search SciFinder-n by References to search for publications by your selected Researcher/*Author Name*. Be sure that your researcher/faculty member is the same person that is currently affiliated with Brock University noting that researchers use an initial or initials or their full name to differentiate themselves, and ORCIC IDs.

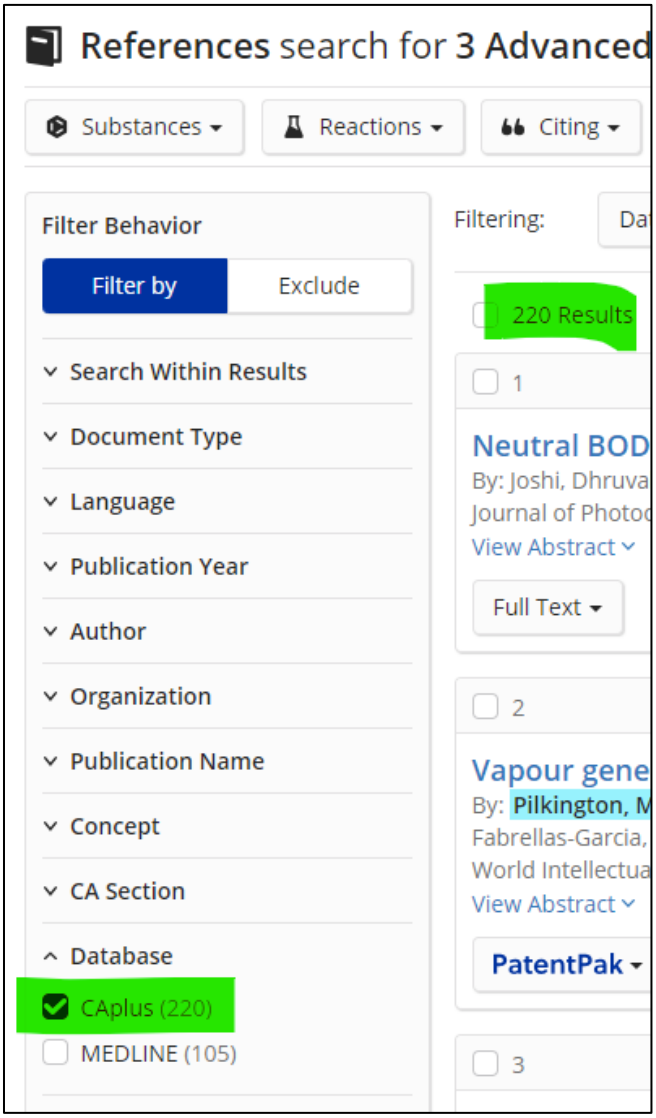
   a. SciFinder-n number of references for this researcher (remember initials, names, etc.): 250, yet when filtered by "Organization" and noting that this researcher has worked with researchers at other universities, institutes… this number is actually less than 250.



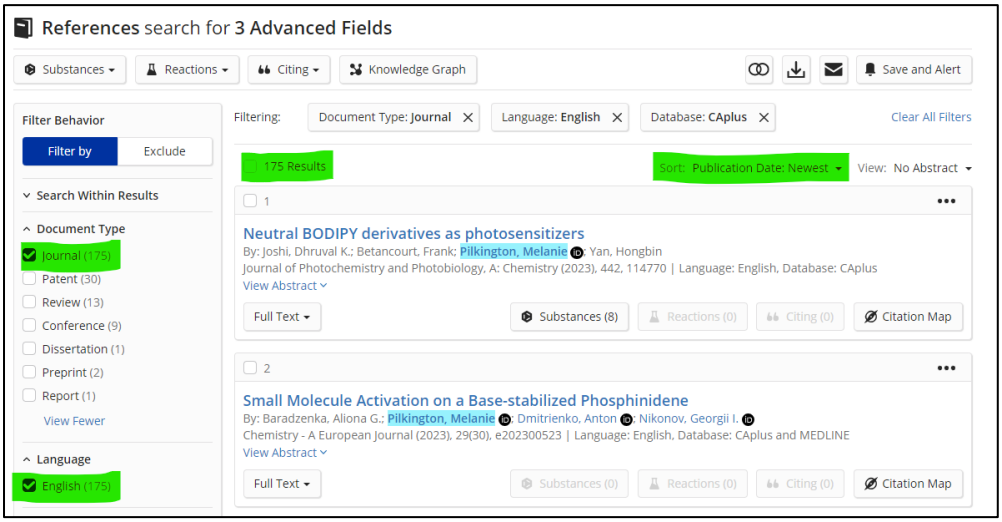
Click on the SciFinder-n Concept filter to have this researcher's work categorized by subject areas. This may help describing your faculty member's subject areas, topics researched and profile.



b. Filter/limit search results for this researcher to find the number of CAplus (Chemical Abstracts) references: 220, note that SciFinder-n searches both MEDLINE and CAplus (Chemical Abstracts) at the same time unless told or filtered differently.



c. Filter References by Document Type = Journal, Language = English, and sort citations by Publication Date: Newest, to find the number of English language scholarly peer-reviewed articles: 175



d. Filter and sort at will to find one recent article of interest that is connected with the work of this course in synthetic organic chemistry. Cite this single article using ACS Style:

Smajlagic, I.; White, B.; Azeez, O.; Pilkington, M.; Dudding, T. Organocatalysis Linked to Charge-Enhanced Acidity with Superelectrophilic Traits. ACS Catal. 2022, 12 (2), 1128–1138. https://doi.org/10.1021/acscatal.1c05296. (journal article)

I use Zotero citation management software (you should as well, get an account, it is free and open!), but for quick references I use Zoterobib and drop in the unique article DOI, and then add "American Chemical Society" when clicking on the "10,000+ other styles available…" link. Cut and paste the citation, and check to make sure it is correctly rendered.

Check out the ACS Quick Style Guide for formatting different types of citations which is Part 4.3 in the ACS Guide to Scholarly Communication. This style guide is constantly updated and comments on all types of scholarship, writing and style. Check it out!

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10.1021/acscatal.1c05296
Cite
Manual Entry
(1) Smajlagic, I.; White, B.; Azeez, O.; Pilkington, M.; Dudding, T. Organocatalysis Linked to Charge-Enhanced Acidity with Superelectrophilic Traits. ACS Catal. 2022, 12 (2), 1128–1138. https://doi.org/10.1021/acscatal.1c05296.
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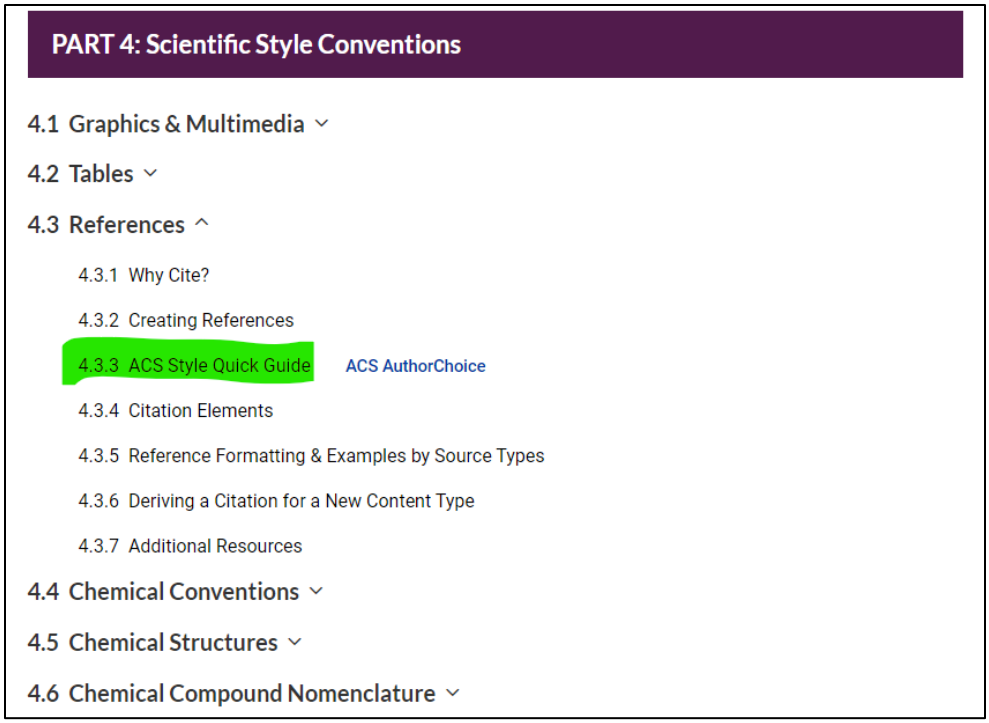
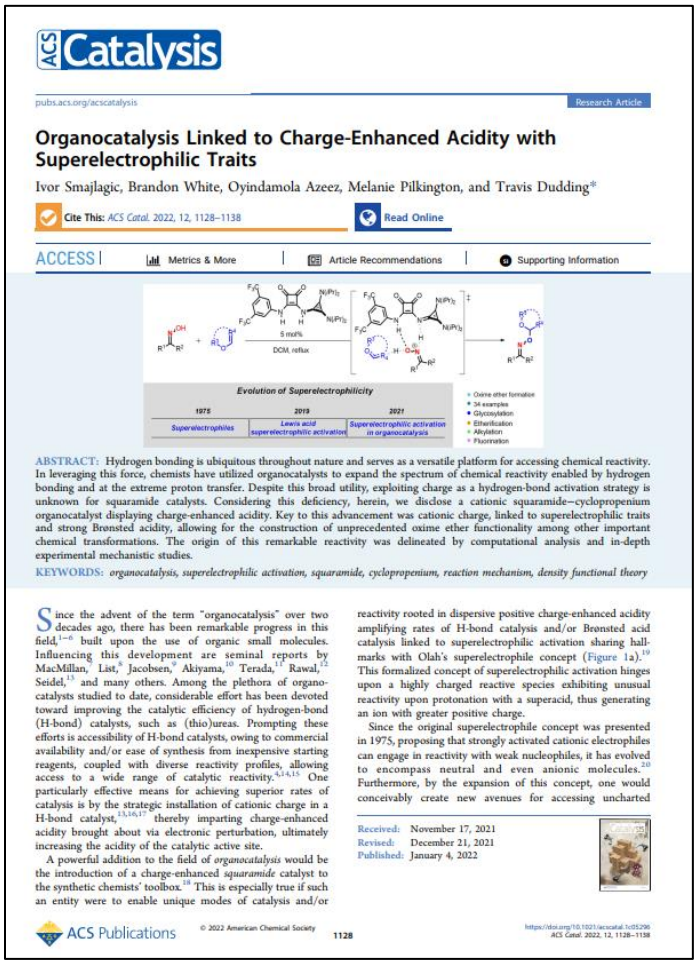

PART 4: Scientific Style Conventions
4.1 Graphics & Multimedia
4.2 Tables
4.3 References
4.3.1 Why Cite?
4.3.2 Creating References
4.3.3 ACS Style Quick Guide
ACS AuthorChoice
4.3.4 Citation Elements
4.3.5 Reference Formatting & Examples by Source Types
4.3.6 Deriving a Citation for a New Content Type
4.3.7 Additional Resources
4.4 Chemical Conventions
4.5 Chemical Structures
4.6 Chemical Compound Nomenclature

Articles from Scientific Journals

Source type	Example
journal article	Foster, J. C.; Varlas, S.; Couturaud, B.; Coe, J.; O'Reilly, R. K. Getting into Shape: Reflections on a New Generation of Cylindrical Nanostructures' Self-Assembly Using Polymer Building Block. *J. Am. Chem. Soc.* **2019**, *141* (7), 2742−2753. DOI: 10.1021/jacs.8b08648
journal article from an aggregator database	Lanzotti A.; Grasso M.; Staiano G.; Martorelli M. The Impact of Process Parameters on Mechanical Properties of Parts Fabricated in PLA with an Open-source 3-D Printer. *Rapid Prototyp. J.* **2015**, *21* (5), 604−617. DOI: 10.1108/RPJ-09-2014-0135 (accessed 2019-11-22 from ProQuest: Materials Science & Engineering Collection).
journal article early publication (article ASAP)	Shang, M.; Ren, M.; Zhou, C. Nitrogen Mustard Induces Formation of DNA−Histone Cross-Links in Nucleosome Core Particles. *Chem. Res. Toxicol.* **2019**, Article ASAP. DOI: 10.1021/acs.chemrestox.9b00354 (accessed 2019-11-21).

Click on the SciFinder-n "Full Text"option and/or cut and paste the article's DOI into OMNI or Brock Library's Google Scholar database (remember to use this account as it is linked to Brock's holdings) to find the full-text PDF copy of this article.

Read it, does it make sense, check out the substances, reactions, acknowledgements, references… create a screen image of the article's and paste the first page into this assignment:



ACS Catalysis

pubs.acs.org/acscatalysis

Research Article

Organocatalysis Linked to Charge-Enhanced Acidity with Superelectrophilic Traits

Ivor Smajlagic, Brandon White, Oyindamola Azeez, Melanie Pilkington, and Travis Dudding*

Cite This: *ACS Catal.* 2022, 12, 1128−1138 | Read Online

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ABSTRACT: Hydrogen bonding is ubiquitous throughout nature and serves as a versatile platform for accessing chemical reactivity. In leveraging this force, chemists have utilized organocatalysts to expand the spectrum of chemical reactivity enabled by hydrogen bonding and at the extreme proton transfer. Despite this broad utility, exploiting charge as a hydrogen-bond activation strategy is unknown for squaramide catalysts. Considering this deficiency, herein, we disclose a cationic squaramide−cyclopropenium organocatalyst displaying charge-enhanced acidity. Key to this advancement was cationic charge, linked to superelectrophilic traits and strong Brønsted acidity, allowing for the construction of unprecedented oxime ether functionality among other important chemical transformations. The origin of this remarkable reactivity was delineated by computational analysis and in-depth experimental mechanistic studies.

KEYWORDS: *organocatalysis, superelectrophilic activation, squaramide, cyclopropenium, reaction mechanism, density functional theory*

Since the advent of the term "organocatalysis" over two decades ago, there has been remarkable progress in this field,[1−6] built upon the use of organic small molecules. Influencing this development are seminal reports by MacMillan,[7] List,[8] Jacobsen,[9] Akiyama,[10] Terada,[11] Rawal,[12] Seidel,[13] and many others. Among the plethora of organocatalysts studied to date, considerable effort has been devoted toward improving the catalytic efficiency of hydrogen-bond (H-bond) catalysts, such as (thio)ureas. Prompting these efforts is accessibility of H-bond catalysts, owing to commercial availability and/or ease of synthesis from inexpensive starting reagents, coupled with diverse reactivity profiles, allowing access to a wide range of catalytic reactivity.[4,14,15] One particularly effective means for achieving superior rates of catalysis is by the strategic installation of cationic charge in a H-bond catalyst,[13,16,17] thereby imparting charge-enhanced acidity brought about via electronic perturbation, ultimately increasing the acidity of the catalytic active site.

A powerful addition to the field of *organocatalysis* would be the introduction of a charge-enhanced *squaramide* catalyst to the synthetic chemists' toolbox.[18] This is especially true if such an entity were to enable unique modes of catalysis and/or reactivity rooted in dispersive positive charge-enhanced acidity amplifying rates of H-bond catalysis and/or Brønsted acid catalysis linked to superelectrophilic activation sharing hallmarks with Olah's superelectrophile concept (Figure 1a).[19] This formalized concept of superelectrophilic activation hinges upon a highly charged reactive species exhibiting unusual reactivity upon protonation with a superacid, thus generating an ion with greater positive charge.

Since the original superelectrophile concept was presented in 1975, proposing that strongly activated cationic electrophiles can engage in reactivity with weak nucleophiles, it has evolved to encompass neutral and even anionic molecules.[20] Furthermore, by the expansion of this concept, one would conceivably create new avenues for accessing uncharted

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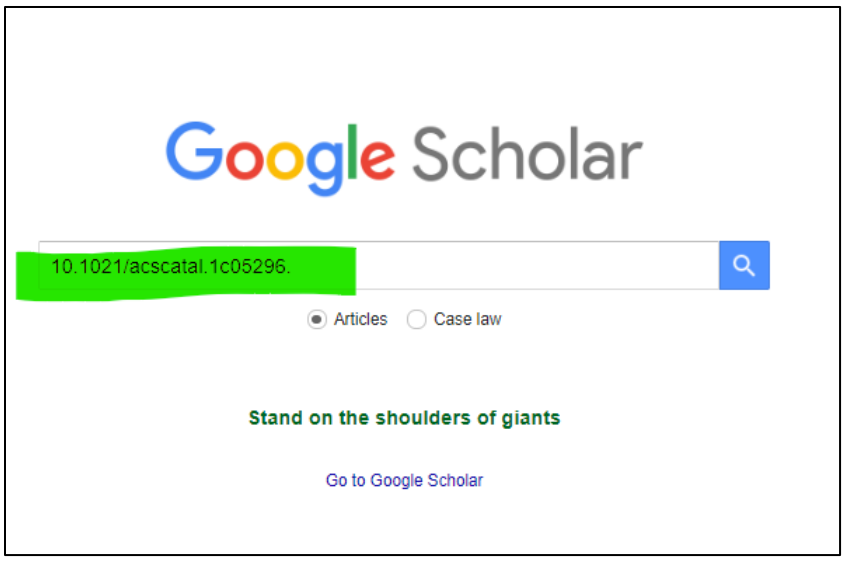
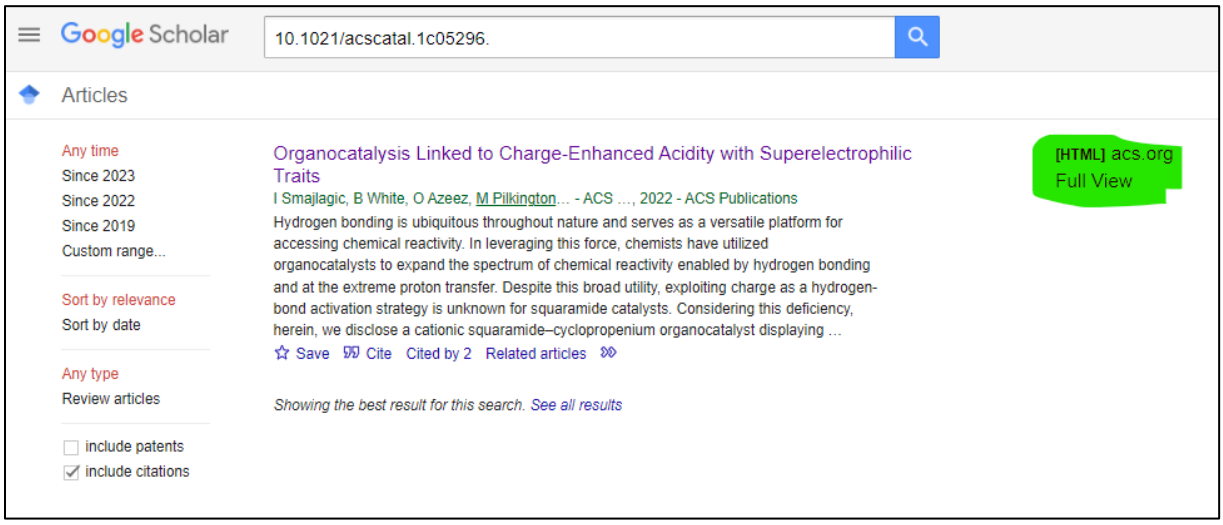
ACS Catal. 2022, 12, 1128−1138

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Sort by date
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Organocatalysis Linked to Charge-Enhanced Acidity with Superelectrophilic Traits
I Smajlagic, B White, O Azeez, M Pilkington... - ACS ..., 2022 - ACS Publications
Hydrogen bonding is ubiquitous throughout nature and serves as a versatile platform for accessing chemical reactivity. In leveraging this force, chemists have utilized organocatalysts to expand the spectrum of chemical reactivity enabled by hydrogen bonding and at the extreme proton transfer. Despite this broad utility, exploiting charge as a hydrogen-bond activation strategy is unknown for squaramide catalysts. Considering this deficiency, herein, we disclose a cationic squaramide–cyclopropenium organocatalyst displaying ...
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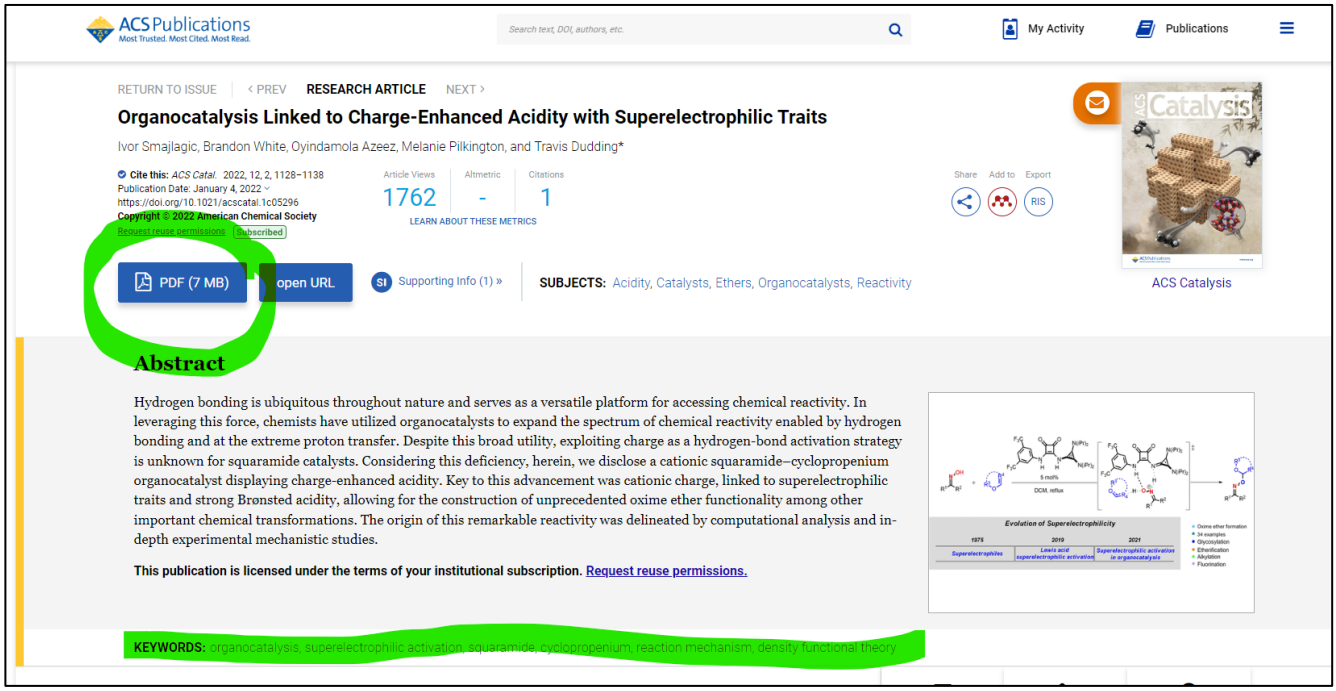
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Organocatalysis Linked to Charge-Enhanced Acidity with Superelectrophilic Traits
Ivor Smajlagic, Brandon White, Oyindamola Azeez, Melanie Pilkington, and Travis Dudding*
Cite this: ACS Catal. 2022, 12, 2, 1128−1138
Publication Date: January 4, 2022
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SI
Supporting Info (1) »
SUBJECTS: Acidity, Catalysts, Ethers, Organocatalysts, Reactivity
ACS Catalysis
Abstract
Hydrogen bonding is ubiquitous throughout nature and serves as a versatile platform for accessing chemical reactivity. In leveraging this force, chemists have utilized organocatalysts to expand the spectrum of chemical reactivity enabled by hydrogen bonding and at the extreme proton transfer. Despite this broad utility, exploiting charge as a hydrogen-bond activation strategy is unknown for squaramide catalysts. Considering this deficiency, herein, we disclose a cationic squaramide−cyclopropenium organocatalyst displaying charge-enhanced acidity. Key to this advancement was cationic charge, linked to superelectrophilic traits and strong Brønsted acidity, allowing for the construction of unprecedented oxime ether functionality among other important chemical transformations. The origin of this remarkable reactivity was delineated by computational analysis and in-depth experimental mechanistic studies.
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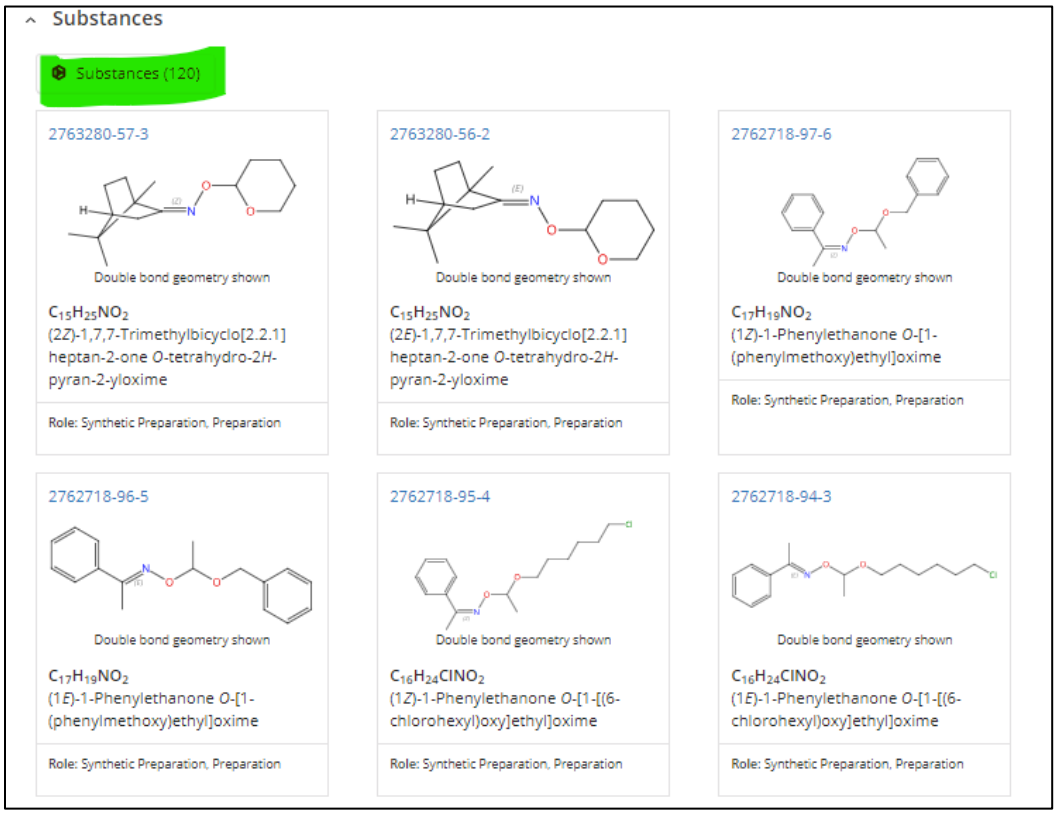
Evolution of Superelectrophilicity
1975
2019
2021
KEYWORDS: organocatalysis, superelectrophilic activation, squaramide, cyclopropenium, reaction mechanism, density functional theory

f. For this SciFinder-n article record the number of database concepts: 33

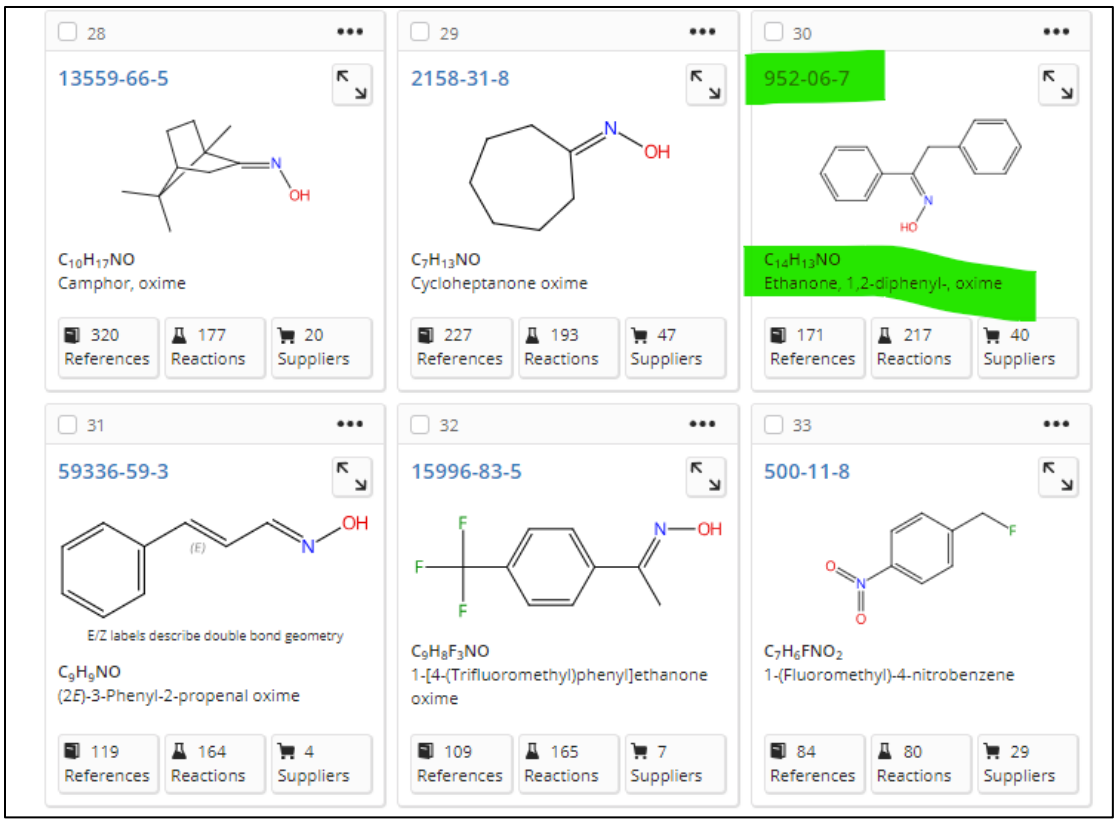
SciFinder-n concepts are ACS database searchable subjects that help to describe an article beyond titles, abstracts, selective substances, reactions, and author's keywords to confirm subject spellings, phrases, roles… and to find alternate articles based on these controlled-language article research descriptors. This helps to think like a chemist when searching and browsing scholarly content.

g. For this SciFinder-n article record the number of unique substances (if available): 120

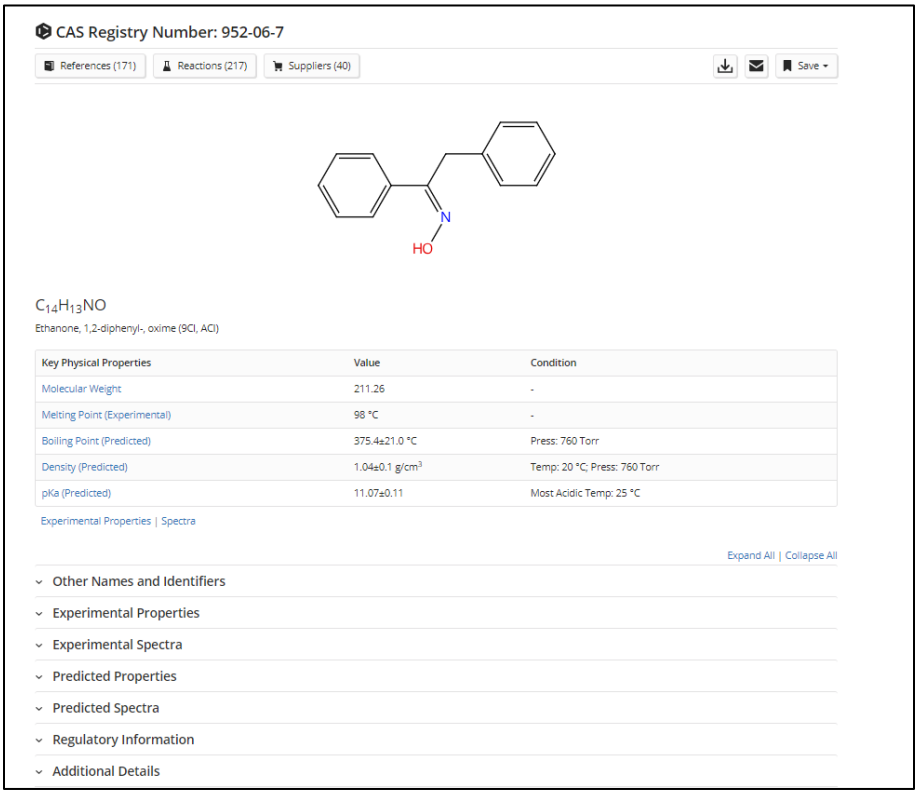
SciFinder-n substances are registered small molecule compounds that describe a single chemical or biological compound. This article involves many different substances and reaction sequences. CAS SciFinder-n captured these substances to help researchers understand this research article. There are many different ways to describe chemicals and biologicals, SciFinder-n uses this database. Click on the "Substances" link to present all chemicals that can be further filtered, added to reactions, sorted, and linked to scholarly references, reactions and suppliers.



h. For this SciFinder-n article select one **organic compound** that is of personal interest, and **has enough references, reactions and suppliers to be noteworthy**. Document the CAS Registry Number you have chosen: 952-06-7

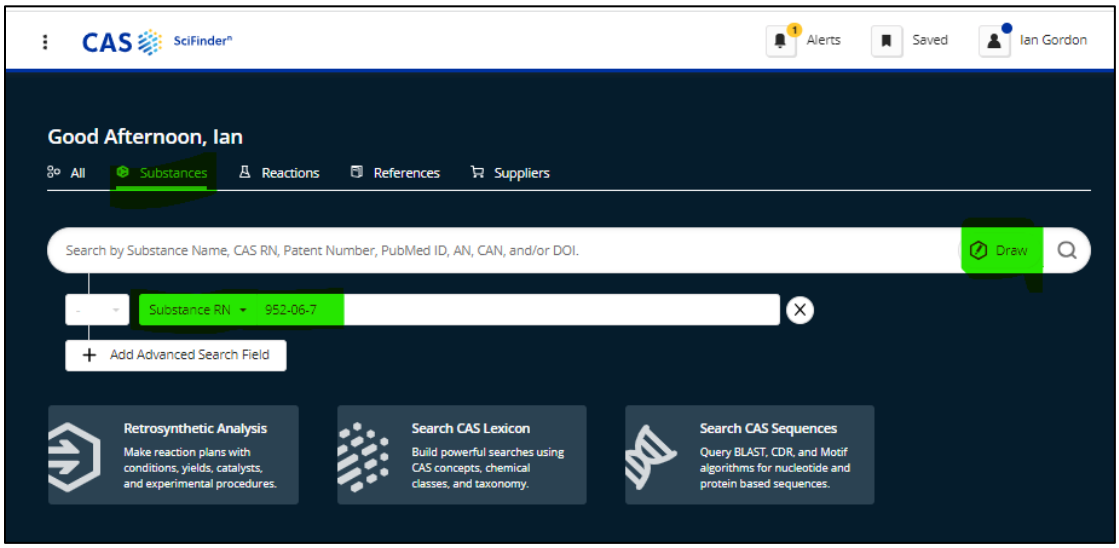


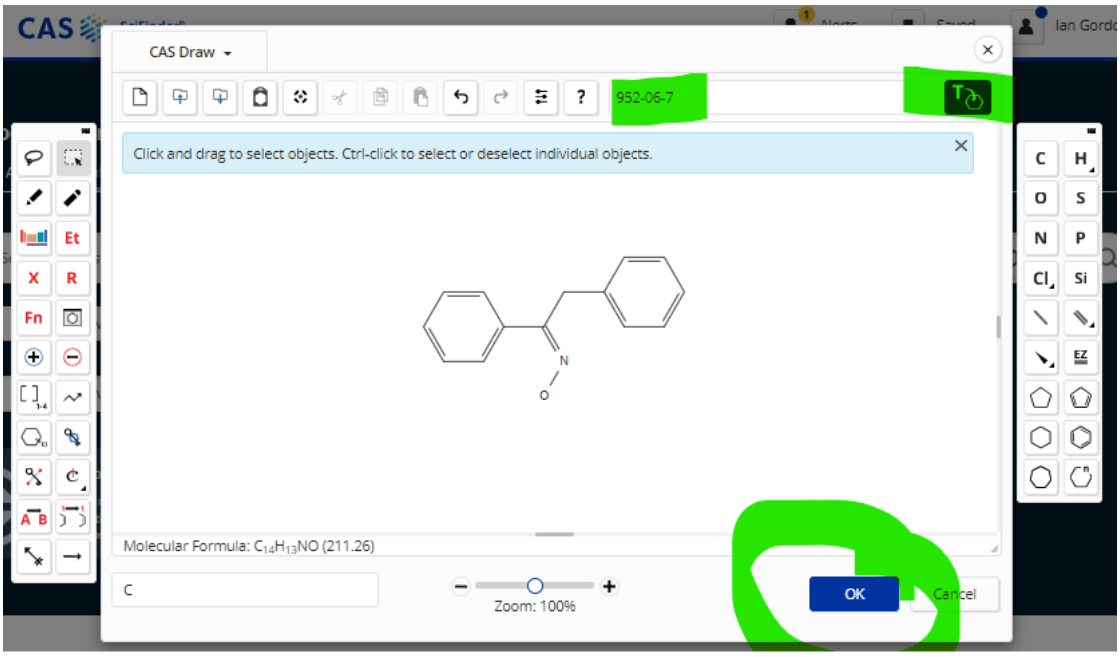
Click on this registry number to learn more about this compound, names, physical properties, and additional details.

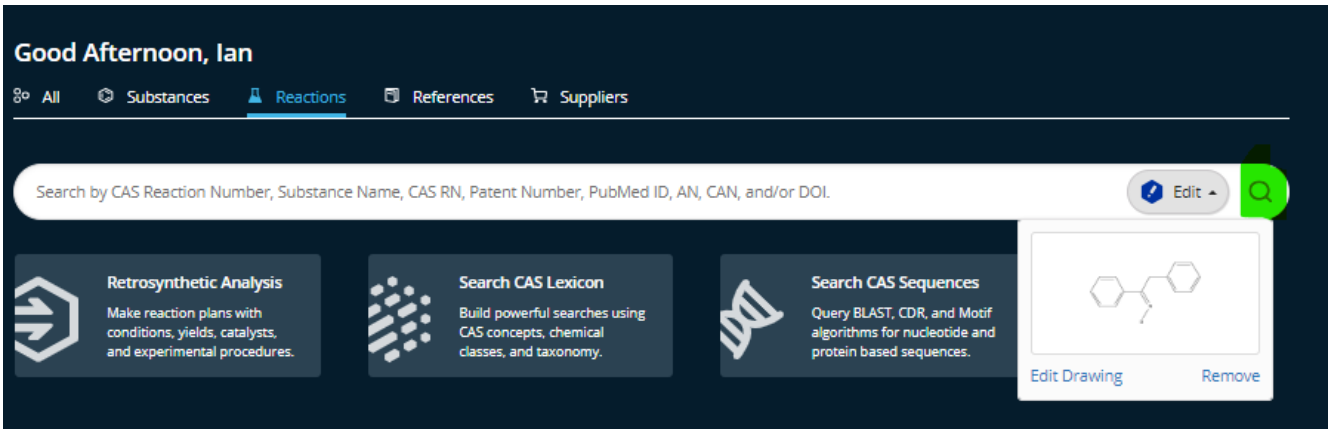

CAS Registry Number: 952-06-7
References (171)
Reactions (217)
Suppliers (40)
Save
$C_{14}H_{13}NO$
Ethanone, 1,2-diphenyl-, oxime (9CI, ACI)
Key Physical Properties | Value | Condition
Molecular Weight | 211.26 | -
Melting Point (Experimental) | 98 °C | -
Boiling Point (Predicted) | 375.4±21.0 °C | Press: 760 Torr
Density (Predicted) | 1.04±0.1 g/cm3 | Temp: 20 °C; Press: 760 Torr
pKa (Predicted) | 11.07±0.11 | Most Acidic Temp: 25 °C
Experimental Properties | Spectra
Expand All | Collapse All
Other Names and Identifiers
Experimental Properties
Experimental Spectra
Predicted Properties
Predicted Spectra
Regulatory Information
Additional Details

5. Chemical structure searching. This is important for organic chemistry and related disciplines. Start a new search and click on SciFinder-n search for Reactions. There are several ways of doing this, click on the SciFinder-n Reactions option, click on the “Draw” icon and insert your CAS Registry number from your previous question. Click on the T search icon next to it, click off to just get the structure and click off “the Click and drag objects…” note. Also note that you can add substances/ structures, short cuts, compounds, reaction sequences… to create a unique structure searching reaction question… For this exercise just click OK. Then click the search icon next to the Draw icon when ready.

   How many substances were found for this drawn structure? 12






Good Afternoon, Ian
All
Substances
Reactions
References
Suppliers
Search by CAS Reaction Number, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI.
Edit
Retrosynthetic Analysis
Make reaction plans with conditions, yields, catalysts, and experimental procedures.
Search CAS Lexicon
Build powerful searches using CAS concepts, chemical classes, and taxonomy.
Search CAS Sequences
Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.
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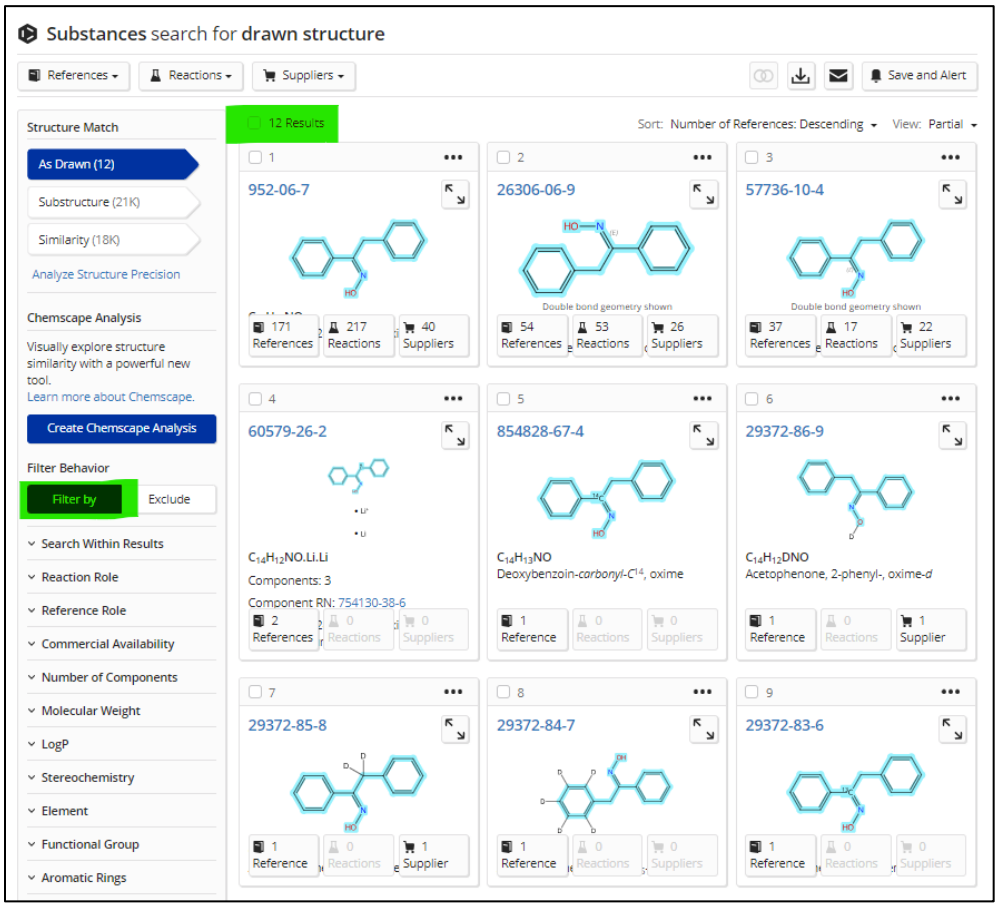
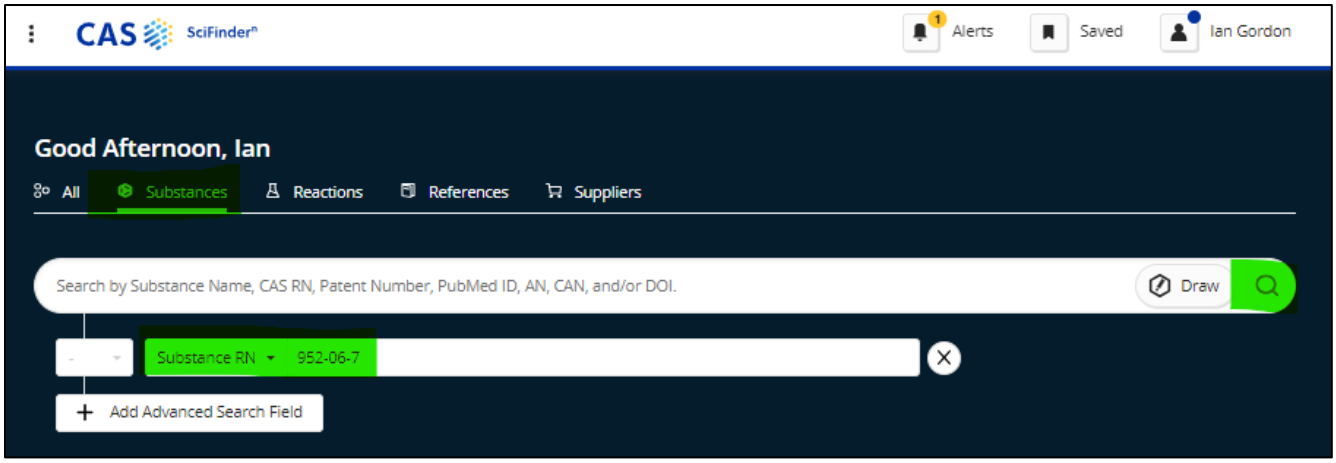
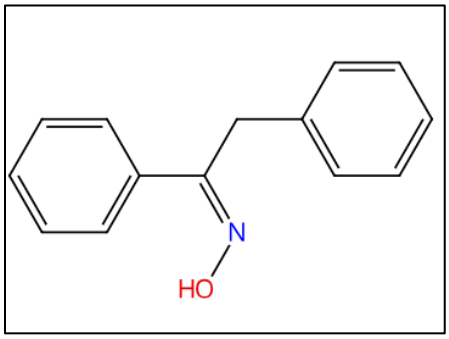


6. Please provide the IUPAC name, registry number and molecular formula (using the Hill system) for your compound identified in question 4h:

   IUPAC chemical name(s) Ethanone, 1,2-diphenyl-, oxime
   CAS Registry Number 952-06-7
   PubChem CID 235383
   molecular formula C14 H13NO

   Copy, cut and paste, or using a chemical drawing software e.g. ChemDraw or create a screen shot of an image or picture of your substance's chemical structure below:





Molecular or chemical formulas are never easy to create, especially for complex, biomolecular, pharmaceuticals, theoretical and trade compounds. There are many different naming conventions, styles and practices. CAS including SciFinder-n build on a specific naming system that is an industry standard, but there are variant names for chemicals, PubChem is another naming convention and open database, see if you compound is found in this database. The Brock Library Chemistry Research Guide is a resource for chemistry and related disciplines, click on the "Chemicals / Drugs" tab to find alternate and open naming databases.

For this SciFinder-n substance, click on Reactions, filter or limit by Substance Role: Product.

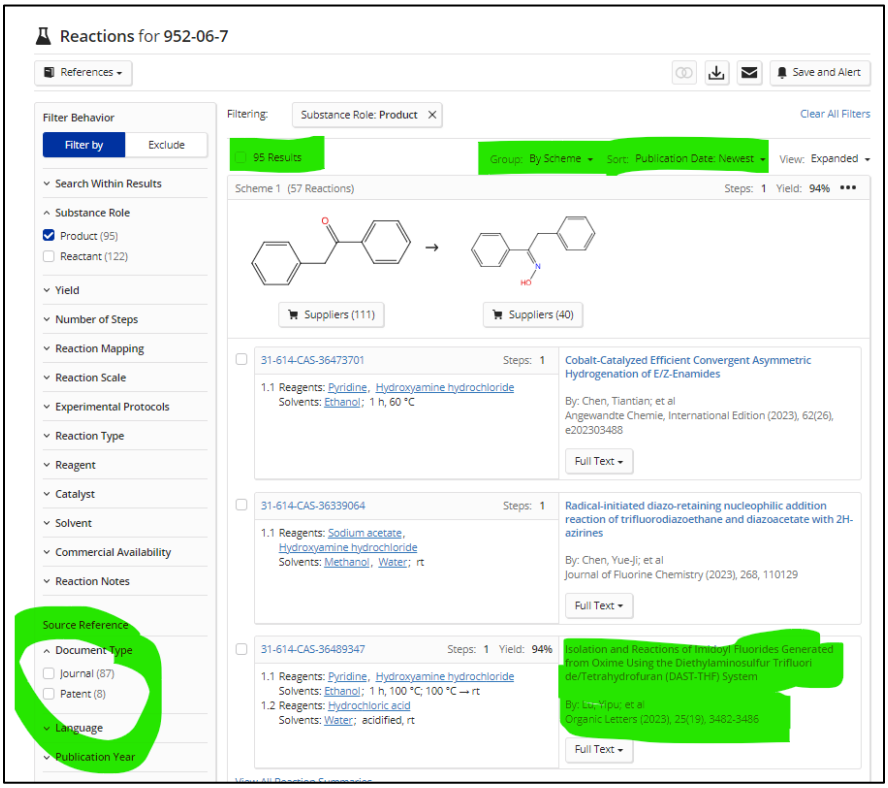
How many reactions as a product are documented in this database? 95

Browse these reactions noting that you can further limit by several variables related to reaction sequences, database filters, document types including journal articles and patents… and sort by several means including relevance, currency, number of steps, yield… and remember that each reaction is cited by at least one scholarly source.

Cite a relevant journal article, then filter by document type: patent - to find a patent. Cite both using ACS Style, (if you can't find a patent then just cite a second article):

Zhao, M.-N. Synthesis of 2,3-Diaryl-2H-Azirines via Cs2CO3-Mediated Cyclization of Ketoxime Acetates. Org. Synth. 2019, 96, 66–79. https://doi.org/10.15227/orgsyn.096.0066. (journal article)

Cho, Li Hwan. Preparation of isothiazole derivatives having antipyretic, analgesic and antiphlogistic activity. US 20040072884, 2004. (patent)



Here is the section of the ACS Check out the ACS Quick Style Guide for formatting different types of citations which is Part 4.3 in the ACS Guide to Scholarly Communication. This style guide is constantly updated and comments on all types of scholarship, writing and style. Here is the patent style example:

patent	Lois-Caballe, C.; Baltimore, D.; Qin, X.-F. Method for Expression of Small RNA Molecules within a Cell. US 7 732 193 B2, 2010.

7. Scholarly Peer Review. Determine whether the article(s) you cited in the previous question is/are peer reviewed.

   What's Peer Review (Brock Library, YouTube, 1:33),

   Are these articles peer reviewed?

   Yes/no Yes

   How do you know? (create our own reply)

   Provides review dates of received, revised, and published on first page, includes references, institutional addresses, methodology and provides new data, results and science/chemistry.

8. Comment: How might accessing SciFinder-n or equivalent scholarly databases help you in this course?

   In a sentence or two, think how this or other chemistry-related disciplinary databases be useful in your program of study.

9. Comment: One thing you learned about the nature of your faculty member's research profile through this exercise?

   In a sentence or two, think how this researcher and their team adds to the body of research in their discipline.

10. Comment: One thing new you learned about SciFinder-n, chemistry databases, and the nature of chemical information through this exercise?

    In a sentence or two, think how chemistry-related disciplinary databases like SciFinder-n differ from other scholarly and AI-aided databases like Google Scholar and might these chemistry database be useful in your program of study.

Help is always available from the Brock Library using Chat with a Librarian, emailing the library using libhelp@brocku.ca, book a research consultation, talking with your lab advisor/TA, talking with colleagues, connecting with chemistry experts using help@cas.org and consulting with any number of disciplinary research guides by program, and the Brock Library Chemistry Research Guide.

Don't forget to sign out of SciFinder-n, remember, and don't share your unique login/password.